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The Softness of the Wills-Harrison Effective Pair Potential in Liquid Fe

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Abstract

It is found that an account of the non-diagonal couplings between *d* electrons sited on different atoms in a transition metal leads to the increase of the softness of repulsive part in the Wills-Harrison effective pair potential for liquid Fe.

Keywords: Transition metal, Wills-Harrison model, *d*-state coupling

In [1] the Wills-Harrison (WH) model [2] was corrected by means the introduction the probability p that all 25 *d*-*d* couplings between two different atoms are equiprobable and probability $(1-p)$ that only 5 equiprobable diagonal couplings are possible. Then, in [1] the WH effective pair potentials, $\varphi_{\mathrm{WH}}(r)$, were considered at different p for liquid Fe, Co and Ni.

Here, we consider how the magnitude p influences the softness of the repulsive part of $\varphi_{\mathrm{WH}}(r)$ for liquid Fe at absolute temperature T=1863K.

The repulsive part of the pair potential $\varphi(r)$ is considered here in the reduced form that is $\beta[\varphi(r)-\varphi(d)]$, where $\beta=1/(k_B T)$, k_{B} - Boltzmann constant, d - position of the first minimum of $\varphi(r)$.

The input parameters of the model are taken from works [2] and [3]. The experimental value of the mean atomic volume equal to 89.29 a.u. is taken from the work [4].

The dependence $\beta[\varphi_{\mathrm{WH}}(r)-\varphi_{\mathrm{WH}}(d)]$ on p is shown in Fig. 1. One can see that the increase of the probability p leads to the increase of the softness of repulsive part in the WH effective pair potential for liquid Fe.

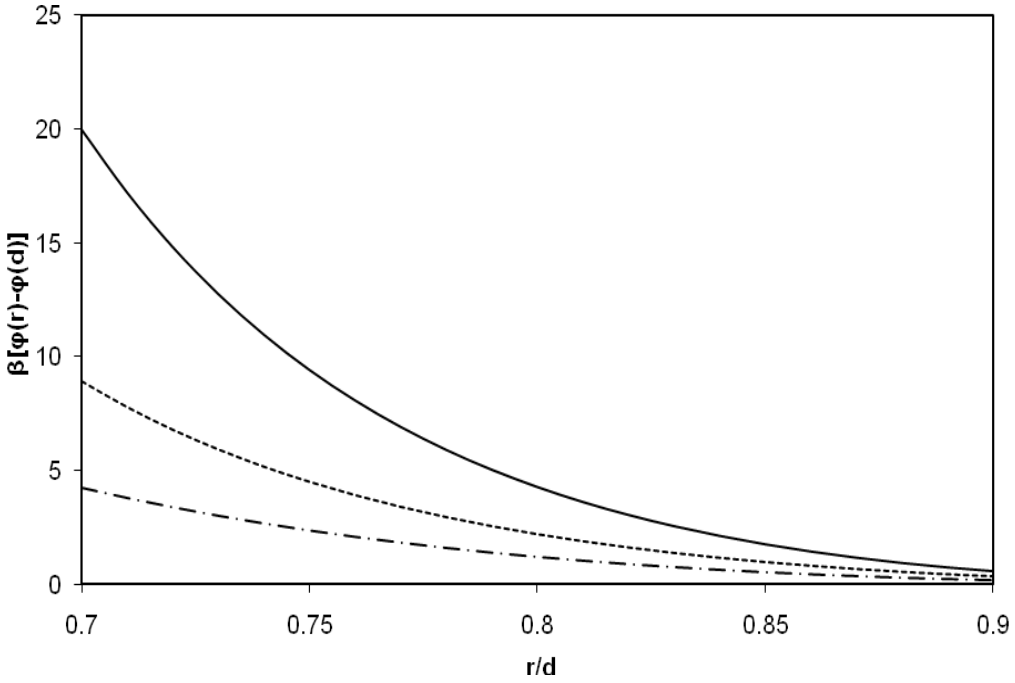

Figure 1. $\beta[\varphi_{\mathrm{WH}}(r)-\varphi_{\mathrm{WH}}(d)]$ in liquid Fe ($p=0$ – solid line; $p=0.5$ – dotted line; $p=1$ – dashed-dotted line).

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